

On the effectiveness of Gamow's method for calculating decay rates

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Abstract

We examine Gamow's method for calculating the decay rate of a wave function initially located within a potential well. Using elementary techniques, we examine a very simple, exactly solvable model, in order to show why it is so reliable for calculating decay rates, in spite of its conceptual problems. We also discuss the regime of validity of the exponential decay law.

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I. INTRODUCTION

Complex-energy “eigenfunctions” made their debut in Quantum Mechanics through the hands of Gamow, in the theory of alpha-decay [1]. Gamow imposed an “outgoing wave boundary condition” on the solutions of the Schrödinger equation for an alpha-particle trapped in the nucleus. Since there is only an *outgoing* flux of alpha-particles, the wavefunction $\psi(r, t)$ must behave far from the nucleus as (for simplicity, we consider an s-wave, and use units such that $\hbar = 2m = 1$)

$$\psi(r, t) \sim \frac{e^{-iEt+ikr}}{r} \quad (r \rightarrow \infty). \quad (1)$$

This boundary condition, together with the requirement of finiteness of the wave function at the origin, gives rise to a quantization condition on the values of k (and, therefore, on the values of $E = k^2$). It turns out that such values are complex:

$$k_n = \kappa_n - iK_n/2, \quad E_n = \epsilon_n - i\Gamma_n/2, \quad (2)$$

and so it follows that

$$|\psi_n(r, t)|^2 \sim \frac{e^{-\Gamma_n t + K_n r}}{r^2} \quad (r \rightarrow \infty). \quad (3)$$

Thus, if $\Gamma_n > 0$, the probability of finding the alpha-particle in the nucleus decays exponentially in time. The lifetime of the nucleus is then given by $\tau_n = 1/\Gamma_n$, and the energy of the emitted alpha-particle by ϵ_n .

Although very natural, this interpretation suffers from some difficulties. How can the energy, which is an observable quantity, be complex? (In other words, how can the Hamiltonian, which is a Hermitean operator, have complex eigenvalues?) Also, these “eigenfunctions” are not normalizable, since Γ_n positive implies K_n positive and so, according to (3), $|\psi_n(r, t)|^2$ diverges exponentially with r .

In spite of such problems (which, in fact, are closely related), it is a fact of life that alpha-decay, as well as other types of decay, does obey an exponential decay law and, in many cases, Gamow’s method provides a very good estimate for the decay rate. Why this method works is a question that has been addressed in the literature using a variety of techniques [2–9]. Here we examine this question in a very elementary way, using techniques that can be found in any standard quantum mechanics textbook and some rudiments of complex analysis.

This paper is structured as follows. In Section II, we show Gamow’s method in action for a very simple potential. Some of the results obtained there are used in Section III, where we study the time evolution of a wave packet initially confined in the potential well defined in Section II. This is done with the help of the propagator, built with the *true* eigenfunctions (i.e., associated to *real* eigenenergies) of the Hamiltonian. As a bonus, we show that the exponential decay law is not valid either for very small or for very large times. This is the content of Section IV, where the region of validity of the exponential decay law is roughly delimited.

II. DECAYING STATES

In order to exhibit Gamow's method in action, we shall study the escape of a particle from the potential well given by:

$$V(x) = \begin{cases} (\lambda/a) \delta(x-a) & \text{for } x > 0, \\ +\infty & \text{for } x < 0. \end{cases} \quad (4)$$

(Escape from this potential well was studied in detail in Refs. [3,8,10]. In this section we follow closely the treatment of Ref. [3].) The positive dimensionless constant λ is a measure of the “opacity” of the barrier at $x = a$; in the limit $\lambda \rightarrow \infty$, the barrier becomes impenetrable, and the energy levels inside the well are quantized. If λ is finite, but large, a particle is not confined to the well anymore, but it usually stays there for a long time before it escapes. If λ is small, the particle can easily tunnel through the barrier, and quickly escape from the potential well. Metastability, therefore, can only be achieved if the barrier is very opaque, i.e., $\lambda \gg 1$. Since this is the most interesting situation, we shall assume this to be the case in what follows.

To find out how fast the particle escapes from the potential well, we must solve the Schrödinger equation

$$i \frac{\partial}{\partial t} \psi(x, t) = -\frac{\partial^2}{\partial x^2} \psi(x, t) + \frac{\lambda}{a} \delta(x-a) \psi(x, t). \quad (5)$$

$\psi(x, t) = \exp(-iEt) \varphi(x)$ is a particular solution of this equation, provided $\varphi(x)$ satisfies the time-independent Schrödinger equation

$$-\frac{d^2}{dx^2} \varphi(x) + \frac{\lambda}{a} \delta(x-a) \varphi(x) = E \varphi(x). \quad (6)$$

Denoting the regions $0 < x < a$ and $x > a$ by the indices 1 and 2, respectively, the corresponding wave functions $\varphi_j(x)$ ($j = 1, 2$) satisfy the free-particle Schrödinger equation:

$$-\frac{d^2}{dx^2} \varphi_j(x) = E \varphi_j(x). \quad (7)$$

Since the wall at the origin is impenetrable, $\varphi_1(0)$ must be zero; the solution of Eq. (7) which obeys this boundary condition is

$$\varphi_1(x) = A \sin kx \quad (k = \sqrt{E}). \quad (8)$$

To determine $\varphi_2(x)$, we follow Gamow's reasoning [1,7,11] and require $\varphi_2(x)$ to be an outgoing wave. Therefore, we select, from the admissible solutions of Eq. (7),

$$\varphi_2(x) = B e^{ikx}. \quad (9)$$

The wave function must be continuous at $x = a$, so that $\varphi_1(a) = \varphi_2(a)$, or

$$\frac{B}{A} = e^{-ika} \sin ka. \quad (10)$$

On the other hand, the derivative of the wave function has a discontinuity at $x = a$, which can be determined by integrating both sides of (6) from $a - \varepsilon$ to $a + \varepsilon$, with $\varepsilon \rightarrow 0^+$:

$$\varphi_2'(a) - \varphi_1'(a) = \frac{\lambda}{a} \varphi_2(a), \quad (11)$$

from which there follows another relation between A and B :

$$\frac{B}{A} = -\frac{ka e^{-ika} \cos ka}{\lambda - ika}. \quad (12)$$

Combining (10) and (12), we obtain a quantization condition for k :

$$ka \cotan ka = -\lambda + ika. \quad (13)$$

The roots of Eq. (13) are complex and situated in the half-plane $\text{Im } k < 0$; when $\lambda \gg 1$, those which are closest to the origin are given by [3,8]

$$k_n a \approx \frac{n\pi\lambda}{1+\lambda} - i \left(\frac{n\pi}{\lambda} \right)^2 \quad (n = 1, 2, \dots; n\pi \ll \lambda). \quad (14)$$

(For each one of these roots, which are located in the fourth quadrant of the complex k -plane, there is a corresponding one in the third quadrant, given by $-k_n^*$. The latter are associated to “growing states” [3] and play no role in what follows.) The corresponding eigenenergies are

$$E_n = k_n^2 \approx \left(\frac{n\pi}{a} \right)^2 - i \frac{2(n\pi)^3}{(\lambda a)^2}. \quad (15)$$

The imaginary part of E_n gives rise to an exponential decay of $|\psi_n(x, t)|^2$, with lifetime equal to

$$\tau_n = 1/\Gamma_n \approx \frac{(\lambda a)^2}{4(n\pi)^3}. \quad (16)$$

Since the corresponding value of B/A is very small ($\sim n/\lambda$), one may be tempted to say that the probability of finding the particle outside the well is negligible in comparison with the probability of finding the particle inside the well. Normalizing ψ_n in such a way that the latter equals one when $t = 0$, the probability of finding the particle inside the well at time t , if it were in the n -th decaying state at $t = 0$, would be

$$P_n(t) = \int_0^a |\psi_n(x, t)|^2 dx = \exp(-\Gamma_n t). \quad (17)$$

The trouble with this interpretation is that $\text{Im } k_n \equiv -K_n/2 < 0$, and so $\psi_n(x, t)$ diverges exponentially as $x \rightarrow \infty$, since, according to (9),

$$|\psi_n(x, t)|^2 = |B_n|^2 \exp(-\Gamma_n t + K_n x) \quad (18)$$

outside the well. Because of this “exponential catastrophe”, the decaying states are non-normalizable and, therefore, cannot be accepted as legitimate solutions of the Schrödinger equation (although one can find in the literature [12] the assertion that they are “rigorous” solutions of the time-dependent Schrödinger equation).

III. TIME EVOLUTION OF A WAVE PACKET

We now return to Eq. (7) and write, for the solution in region 2, instead of (9), the sum of an outgoing plus an incoming wave:

$$\varphi_2(x) = e^{-ikx} + B e^{ikx}. \quad (19)$$

Continuity of the wave function at $x = a$ implies

$$A \sin ka = e^{-ika} + B e^{ika}. \quad (20)$$

As before, the derivative of the wave function has a discontinuity at $x = a$, given by Eq. (11), from which it follows, instead of (12),

$$kA \cos ka = -\left(\frac{\lambda}{a} + ik\right) e^{-ika} - \left(\frac{\lambda}{a} - ik\right) B e^{ika}. \quad (21)$$

Solving (20) and (21) for A and B , we find

$$A(k) = -\frac{2ika}{ka + \lambda e^{ika} \sin ka}, \quad (22a)$$

$$B(k) = -\frac{ka + \lambda e^{-ika} \sin ka}{ka + \lambda e^{ika} \sin ka}. \quad (22b)$$

These expressions show a couple of interesting features:

- $|B| = 1$ for real values of k , implying a zero net flux of probability through $x = a$; therefore, unlike the solution found in the previous section, there is no loss or accumulation of probability in the well region.
- $|A| \ll 1$ if $ka \ll \lambda$, except if k is close to a pole of $A(k)$, in which case $|A|$ may become very large.

To find the poles of A we must solve the equation $A(k)^{-1} = 0$, which, after some algebraic manipulations, reads

$$ka \cotan ka = -\lambda + ika. \quad (23)$$

This is the same as Eq. (13)! Is this a coincidence? In fact, no. According to (22), A and B have the same poles; therefore, near a pole both $|A|$ and $|B|$ are very large, and Eqs. (20) and (21) become equivalent to Eqs. (10) and (12), respectively. In what follows, we shall show that the poles of A (and B) play an important role in the decay process.

Suppose that at $t = 0$ the particle is known to be in the region $x < a$ with probability 1; in other words, its wave function $\psi(x, 0)$ is zero outside the well. Then, at a later time t , the wave function is given by

$$\psi(x, t) = \int_0^a G(x, x'; t) \psi(x', 0) dx', \quad (24)$$

where the propagator, $G(x, x'; t)$, can be written as

$$G(x, x'; t) = \int_0^\infty e^{-ik^2 t} \varphi_k(x) \varphi_k^*(x') dk. \quad (25)$$

The function $\varphi_k(x)$ is the solution of Eq. (6) corresponding to the energy $E = k^2$:

$$\varphi_k(x) = \frac{1}{\sqrt{2\pi}} \times \begin{cases} A(k) \sin kx & \text{for } x < a, \\ e^{-ikx} + B(k) e^{ikx} & \text{for } x > a. \end{cases} \quad (26)$$

With this normalization, these functions satisfy the completeness relation [13]

$$\int_0^\infty \varphi_k(x) \varphi_k^*(x') dk = \delta(x - x'). \quad (27)$$

Eqs. (24)–(26) give, for $x < a$,

$$\psi(x, t) = \frac{1}{2\pi} \int_0^\infty e^{-ik^2 t} \phi(k) |A(k)|^2 \sin kx dk, \quad (28)$$

where

$$\phi(k) \equiv \int_0^a \psi(x', 0) \sin kx' dx'. \quad (29)$$

It is clear that the integral over k is dominated by the resonances, i.e., the neighborhood of the poles of $A(k)$.

Since, for $t > 0$, $e^{-ik^2 t} \rightarrow 0$ when $|k| \rightarrow \infty$ in the fourth quadrant, one can rotate¹ the integration contour by 45° in the clockwise sense (see Fig. 1), thus obtaining

$$\psi(x, t) = e^{-i\pi/4} \int_0^\infty e^{-k^2 t} f(e^{-i\pi/4} k, x) dk + \sum_{n=1}^\infty C(k_n, x) e^{-ik_n^2 t}, \quad (30)$$

where

$$f(k, x) \equiv \frac{1}{2\pi} \phi(k) |A(k)|^2 \sin kx \quad (31)$$

and

$$C(k_n, x) = -2\pi i \lim_{k \rightarrow k_n} (k - k_n) f(k, x). \quad (32)$$

The sum in (30) takes into account the poles of $A(k)$ which are situated in the region $-\pi/4 < \arg k < 0$, and it corresponds to an expansion in Gamow states (for $x < a$).

Let us put aside, for a moment, the integral in (30) (it will be discussed in the next section). Then, the “nonescape” probability (i.e., the probability of finding the particle inside the well) is given by

¹For this to be possible $\phi(k)$ must be an analytic function of k , but this can be shown to be the case [14] if $\psi(x', 0)$ is continuous in $[0, a]$.

$$P(t) = \int_0^a |\psi(x, t)|^2 dx \approx \sum_{n=1}^{\infty} c_n e^{-\Gamma_n t} + \text{interference terms}, \quad (33)$$

where $c_n \equiv \int_0^a |C(k_n, x)|^2 dx$. For $\lambda \gg 1$, the interference terms are usually negligible, for $k_n \approx n\pi/a$ and, therefore, the functions $C(k_n, x) \propto \sin k_n x$ are approximately orthogonal. On the other hand, since the decay rate Γ_n of the n -th decaying mode is a rapidly increasing function of n ($\Gamma_n \approx n^3 \Gamma_1$), the decay becomes almost a pure exponential one when $\Gamma_1 t \gtrsim 1$. The system, therefore, “loses memory” of the initial state.

Finally, let us note that no exponential catastrophe occurs with $\psi(x, t)$. In fact, one can easily show, using (24), (25), (27) and the orthogonality of the eigenfunctions $\varphi_k(x)$, that

$$\int_0^{\infty} |\psi(x, t)|^2 dx = \int_0^{\infty} |\psi(x, 0)|^2 dx, \quad (34)$$

so that an exponential growth of $|\psi(x, t)|^2$ is completely ruled out.

IV. BREAKDOWN OF EXPONENTIAL DECAY

In order to derive expression (33) for the nonescape probability, we had to neglect the first term on the right hand side of (30). In this section we show that such approximation is not valid either for very small or for very large times. That it cannot be valid for very small t follows from the fact that initially the decay is slower than exponential [4,5]. This can be easily proved with the help of the continuity equation [15]:

$$\frac{d}{dt} P(t) = -\frac{\hbar}{m} \text{Im} \left[\psi(x, t) \frac{\partial}{\partial x} \psi^*(x, t) \right]_{x=a}. \quad (35)$$

Since, by hypothesis, $\psi(a, 0) = 0$, it follows that $dP/dt = 0$ when $t = 0$, whereas for the expression (33) one has $dP/dt \approx -\sum c_n \Gamma_n < 0$ at $t = 0$.

On the other hand, the exponential decay does not last forever. After a sufficiently long time, it obeys a power law [2–5,8,16]. To see this, note that the integral in (30), which we shall denote here by $I(x, t)$, is dominated by small values of k when $t \rightarrow \infty$, and so can it be approximated by

$$I(x, t) \approx \frac{e^{-i\pi/4}}{2\pi} \phi'(0) |A(0)|^2 x \int_0^{\infty} k^2 e^{-k^2 t} dk \sim \frac{a^{3/2} x}{\lambda^2 t^{3/2}} \quad (36)$$

Therefore, the nonescape probability behaves asymptotically as²

$$P(t) \approx \int_0^a |I(x, t)|^2 dx \sim \frac{a^6}{\lambda^4 t^3}. \quad (37)$$

²García-Calderón, Mateos and Moshinsky [8] argue that the nonescape probability $P(t)$ decays as t^{-1} when $t \rightarrow \infty$, in contrast to Eq. (37). However, there is a flaw in their argument; when properly corrected [17], it also leads to $P(t) \sim t^{-3}$ asymptotically.

Comparing (37) with (33), and using (16), one finds that they become comparable in magnitude when

$$e^{-t/\tau_1} \sim \frac{a^6}{\lambda^4 t^3} \sim \lambda^{-10} \left(\frac{\tau_1}{t} \right)^3, \quad (38)$$

or, since $\lambda \gg 1$, when

$$\frac{t}{\tau_1} \sim 10 \ln \lambda. \quad (39)$$

In practice, when the decay begins to obey a power law the nonescape probability is so small ($\sim \lambda^{-10}$) that it should be very difficult to observe deviations from exponential decay. (On the other hand, experimental evidence for non-exponential decay at *small* times has been reported recently [18].)

In closing this section, we would like to remark that the breakdown of the exponential decay law for either small or large times is not a peculiar feature of the potential (4). It is possible to show that an exponential decay cannot last forever if the Hamiltonian is bounded below [19,4,5], and cannot occur for very small times if, besides that, the energy expectation value of the initial state is finite [4,5] — conditions which certainly must be satisfied by any realistic Hamiltonian or state.

V. CONCLUSION

In this paper we showed that decaying states, although plagued by the exponential catastrophe, give a fairly good description of the decay of a metastable state, provided some conditions are satisfied. In fact, the main objective of this paper was to show that one *can* compute the decay rate solving the time independent Schrödinger equation subject to the “outgoing wave boundary condition.” This is far from being a trivial result, since the corresponding eigenstates are unphysical. The effectiveness of the decaying states in describing the decay may be understood by noticing [6] that they are good approximate solutions to the time-dependent Schrödinger equation, although nonuniform ones (i.e., they are not valid in the entire range of values of t and x).

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FIGURES

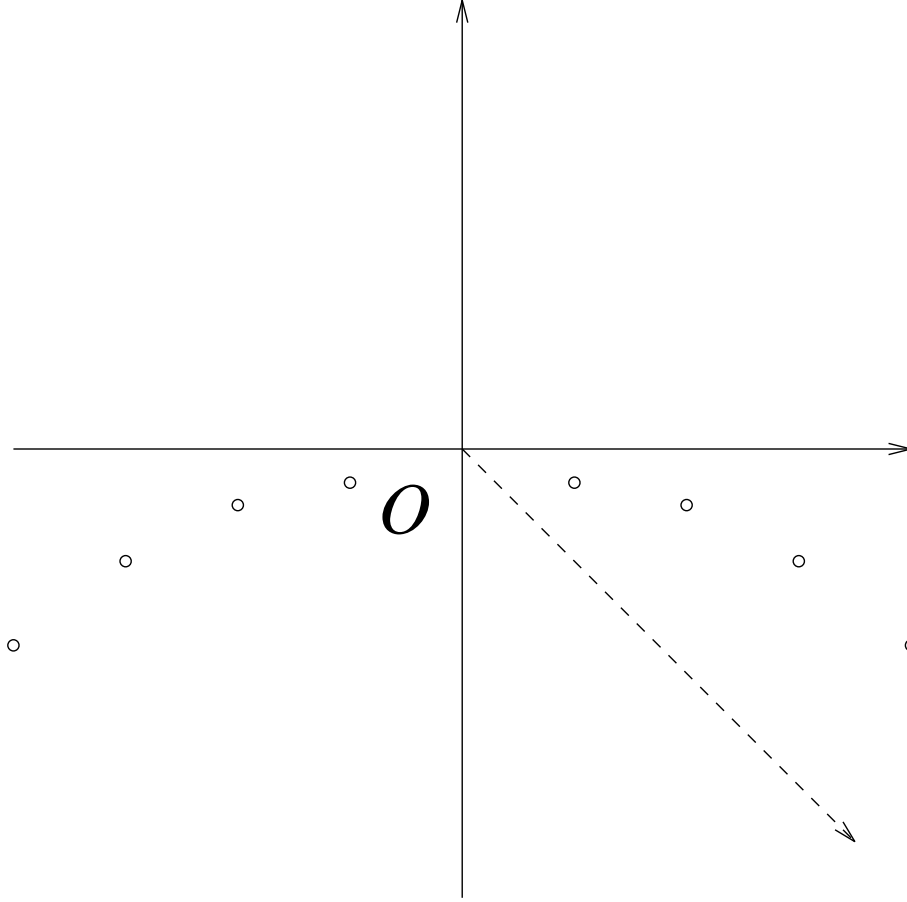


FIG. 1. Complex k -plane. The poles of $A(k)$ are represented by the small circles. Those in the fourth quadrant give rise to the sum over decaying modes in Eq. (30) when one rotates the integration contour of Eq. (28) — the positive real semi-axis — by 45° in the clockwise sense (dashed line).